Determinations of upper critical field in the c-a plane

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Within a continuous Ginzburg-Landau model for layered superconductors, two procedures are proposed to determine the upper critical field parallel to the c-a crystal plane with an angle θ tilted from the c-axis. For an intrinsically layered superconductor, the upper critical fields for $\theta \to 90°$, as determined by the two procedures, are consistent with each other and in reasonably good agreement with those determined by similar procedures suited for the parallel upper critical field ($\theta = 90°$). The profile of the order parameter obtained at B_{c2} is Gaussian-like, indicating the plausibility of the procedures proposed.

I. INTRODUCTION

Theories within the Ginzburg-Landau (GL) framework are important for studies of properties of layered superconductors. Considering the layered structure of high T_c superconductors (HTSs), Koyama *et al.*[1] first proposed a continuous Ginzburg-Landau (CGL) model, in which the GL coefficients and the superpair masses are spatially dependent. Recently, we have proposed a similar CGL model and have applied it to a layered superconductor without a magnetic field[2], and to layered systems with a magnetic field parallel to the a- (b-) crystal axis[3]. Details of the determinations of the parallel upper critical field

were given in Ref. 4. In this work, our CGL formulation is applied to layered superconductors immersed in a magnetic field parallel to the c-a crystal plane. Two procedures shall be proposed to determine the upper critical field, which is a subject of long-term interest[5].

II. MODEL

We consider a layered superconductor comprising of alternating superconducting (S) and insulating (I) layers along the c-axis. The CGL free energy for the system is[2],

$$F = \int d\vec{r} \int dz \left[\alpha(T,z)|\Psi(\vec{r},z)|^2 + \frac{1}{2}\beta|\Psi(\vec{r},z)|^4 + \frac{\hbar^2}{2M(z)} \left| \left(\frac{\partial}{\partial z} - \frac{2ie}{\hbar}A_z(\vec{r},z) \right) \Psi(\vec{r},z) \right|^2 \right.$$
$$\left. + \frac{\hbar^2}{2m(z)} \left| \left(\nabla^{(2)} - \frac{2ie}{\hbar}\vec{A}^{(2)}(\vec{r},z) \right) \Psi(\vec{r},z) \right|^2 + \frac{1}{2\mu_0}B^2(\vec{r},z) \right], \tag{1}$$

where $\vec{r} = (x,y)$ is the planar vector and $\vec{A}(\vec{r},z) = (\vec{A}^{(2)}(\vec{r},z), A_z(\vec{r},z))$ is the vector potential. $\Psi(\vec{r},z)$ is the superconducting order parameter and $B(\vec{r},z)$ is the internal magnetic field. β is assumed constant[2,6]. The CGL condensation coefficient $\alpha(T,z)$ and the perpendicular and parallel effective masses, $M(z)$ and $m(z)$, are assumed as before[2,3]:

$$\alpha(T,z) = [\alpha_0 + \alpha_1 \cos(2\pi z/D)]\,(1 - T/T_c), \tag{2a}$$

$$\frac{1}{M(z)} = G_0 + G_1 \cos(2\pi z/D), \tag{2b}$$

$$\frac{1}{m(z)} = g_0 + g_1 \cos(2\pi z/D), \tag{2c}$$

where α_0, α_1, G_0, G_1, g_0 and g_1 are the model parame-

ters. D is the size of the unit cell equal to $d_I/2 + d_S + d_I/2 = d_I + d_S$, with d_I and d_S denoting the thickness of the I and S layers, respectively. In the present simulation for layered superconductors, the intrinsically layered cuprate $Bi_2Sr_2CaCu_2O_8$ (Bi2212) is chosen as the modeling prototype as this superconductor has an explicitly layered structure due to its high anisotropy[7]. Details of the calculation inputs for Bi2212 can be found in Ref. 3.

Let us now consider the case where an external magnetic field B is applied in the direction tilted from the z-axis (c-axis) by an angle θ in the z-x (c-a) plane. Taking the vector potential as $\vec{A} = (0, B(x\cos\theta - z\sin\theta), 0)$, the linearized CGL equation from the CGL free energy is obtained as follows,

$$-\frac{\hbar^2}{2M(z)}\frac{\partial^2}{\partial z^2}\Psi(x,y,z) - \frac{\hbar^2}{2}\left[\frac{\partial}{\partial z}\frac{1}{M(z)}\right]\frac{\partial}{\partial z}\Psi(x,y,z)$$
$$-\frac{\hbar^2}{2m(z)}\left[\frac{\partial^2}{\partial x^2} + \left(\frac{\partial}{\partial y} - 2ieB(x\cos\theta - z\sin\theta)\right)^2\right]\Psi(x,y,z) + \alpha(T,z)\Psi(x,y,z) = 0. \tag{3}$$

In a new coordinate system,

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \tag{4}$$

Eq. 3 becomes

$$-\frac{\hbar^2}{2M(x',z')}\left(-\sin\theta\frac{\partial}{\partial x'} + \cos\theta\frac{\partial}{\partial z'}\right)^2 \Psi(x',y',z')$$

$$-\frac{\hbar^2}{2}\left[\left(-\sin\theta\frac{\partial}{\partial x'} + \cos\theta\frac{\partial}{\partial z'}\right)\frac{1}{M(x',z')}\right]\left(-\sin\theta\frac{\partial}{\partial x'} + \cos\theta\frac{\partial}{\partial z'}\right)\Psi(x',y',z')$$

$$-\frac{\hbar^2}{2m(x',z')}\left[\left(\cos\theta\frac{\partial}{\partial x'} + \sin\theta\frac{\partial}{\partial z'}\right)^2 + \left(\frac{\partial}{\partial y'} - 2ieBx'\right)^2\right]\Psi(x',y',z')$$

$$+\,\alpha(T,x',z')\Psi(x',y',z') = 0. \tag{5}$$

Assuming $\Psi(x',y',z') = e^{iky'}\Phi(x',z')$, it follows from Eq. 5 that

$$-\frac{\hbar^2}{2M(x',z')}\left(-\sin\theta\frac{\partial}{\partial x'} + \cos\theta\frac{\partial}{\partial z'}\right)^2 \Phi(x',z')$$

$$-\frac{\hbar^2}{2}\left[\left(-\sin\theta\frac{\partial}{\partial x'} + \cos\theta\frac{\partial}{\partial z'}\right)\frac{1}{M(x',z')}\right]\left(-\sin\theta\frac{\partial}{\partial x'} + \cos\theta\frac{\partial}{\partial z'}\right)\Phi(x',z')$$

$$-\frac{\hbar^2}{2m(x',z')}\left[\left(\cos\theta\frac{\partial}{\partial x'} + \sin\theta\frac{\partial}{\partial z'}\right)^2 - 4e^2B^2(x'-x_0')^2\right]\Phi(x',z')$$

$$+\,\alpha(T,x',z')\Phi(x',z') = 0, \tag{6}$$

with $x_0' = \hbar k/(2eB)$. For $0 \le \theta < 90°$, one may choose $x_0' = 0$[8].

For a given temperature T, the maximum magnetic field B which satisfies Eq. 6 gives a point on the B_{c2}-T plot. Eq. 6 shall be numerically solved subject to the following boundary conditions[8],

$$\Phi(x',0) = \Phi(x',D/\cos\theta), \tag{7a}$$

$$\frac{\partial}{\partial z'}\Phi(x',z')|_{z'=0} = \frac{\partial}{\partial z'}\Phi(x',z')|_{z'=D/\cos\theta}, \tag{7b}$$

$$\Phi(x',z')|_{x'\to\pm\infty} = 0. \tag{7c}$$

III. NUMERICAL PROCEDURES

A. Procedure I

Taken into account the boundary conditions, Eq. 6 can be represented as

$$\mathbf{U\Phi} = \mathbf{0}, \tag{8}$$

where the column vector $\mathbf{\Phi} = \{\Phi_k\}'$, $k = 1,2,...,(2n-2)\times 2n$ represents the discrete solutions of Eq. 6 (here $'$ indicates transpose, k and n are integers). The sparse matrix $\mathbf{U}$ has the following structure,

$$\mathbf{U} = \begin{pmatrix} \mathbf{U}_{3,2} & \mathbf{U}_{4,2} & \mathbf{U}_{5,2} & & & & \\ \mathbf{U}_{2,3} & \mathbf{U}_{3,3} & \mathbf{U}_{4,3} & \mathbf{U}_{5,3} & & & \\ \mathbf{U}_{1,4} & \mathbf{U}_{2,4} & \mathbf{U}_{3,4} & \mathbf{U}_{4,4} & \mathbf{U}_{5,4} & & \\ & \mathbf{U}_{1,5} & \mathbf{U}_{2,5} & \mathbf{U}_{3,5} & \mathbf{U}_{4,5} & \mathbf{U}_{5,5} & \\ & & & \ddots & & & \\ & & \mathbf{U}_{1,2n-4} & \mathbf{U}_{2,2n-4} & \mathbf{U}_{3,2n-4} & \mathbf{U}_{4,2n-4} & \mathbf{U}_{5,2n-4} \\ & & & \mathbf{U}_{1,2n-3} & \mathbf{U}_{2,2n-3} & \mathbf{U}_{3,2n-3} & \mathbf{U}_{4,2n-3} & \mathbf{U}_{5,2n-3} \\ & & & & \mathbf{U}_{1,2n-2} & \mathbf{U}_{2,2n-2} & \mathbf{U}_{3,2n-2} & \mathbf{U}_{4,2n-2} \\ & & & & & \mathbf{U}_{1,2n-1} & \mathbf{U}_{2,2n-1} & \mathbf{U}_{3,2n-1} \end{pmatrix}, \tag{9}$$

where the block matrices $\mathbf{U}_{l,i}$ ($l = 1, 2, 3, 4, 5$) can be expressed as follows

$$\mathbf{U}_{1,i} = \begin{pmatrix} 0 & & & & & & & & 0 \\ c_{2,i,2} & c_{3,i,2} & c_{4,i,2} & c_{5,i,2} & & & & c_{1,i,2} & \\ c_{1,i,3} & c_{2,i,3} & c_{3,i,3} & c_{4,i,3} & c_{5,i,3} & & & & \\ & c_{1,i,4} & c_{2,i,4} & c_{3,i,4} & c_{4,i,4} & c_{5,i,4} & & & \\ & & & \ddots & & & & & \\ & & & c_{1,i,2n-3} & c_{2,i,2n-3} & c_{3,i,2n-3} & c_{4,i,2n-3} & c_{5,i,2n-3} & \\ & & & & c_{1,i,2n-2} & c_{2,i,2n-2} & c_{3,i,2n-2} & c_{4,i,2n-2} & c_{5,i,2n-2} \\ & c_{5,i,2n-1} & & & & c_{1,i,2n-1} & c_{2,i,2n-1} & c_{3,i,2n-1} & c_{4,i,2n-1} \\ 0 & & & & & & & & 0 \end{pmatrix}, \tag{10}$$

$$\mathbf{U}_{2,i} = \begin{pmatrix} 0 & & & & & & & & 0 \\ c_{7,i,2} & c_{8,i,2} & c_{9,i,2} & c_{10,i,2} & & & & c_{6,i,2} & \\ c_{6,i,3} & c_{7,i,3} & c_{8,i,3} & c_{9,i,3} & c_{10,i,3} & & & & \\ & c_{6,i,4} & c_{7,i,4} & c_{8,i,4} & c_{9,i,4} & c_{10,i,4} & & & \\ & & & \ddots & & & & & \\ & & & c_{6,i,2n-3} & c_{7,i,2n-3} & c_{8,i,2n-3} & c_{9,i,2n-3} & c_{10,i,2n-3} & \\ & & & & c_{6,i,2n-2} & c_{7,i,2n-2} & c_{8,i,2n-2} & c_{9,i,2n-2} & c_{10,i,2n-2} \\ & c_{10,i,2n-1} & & & & c_{6,i,2n-1} & c_{7,i,2n-1} & c_{8,i,2n-1} & c_{9,i,2n-1} \\ 0 & & & & & & & & 0 \end{pmatrix}, \tag{11}$$

$$\mathbf{U}_{3,i} = \begin{pmatrix} 1 & & & & & & & & -1 \\ c_{12,i,2} & c_{13,i,2} & c_{14,i,2} & c_{15,i,2} & & & & c_{11,i,2} & \\ c_{11,i,3} & c_{12,i,3} & c_{13,i,3} & c_{14,i,3} & c_{15,i,3} & & & & \\ & c_{11,i,4} & c_{12,i,4} & c_{13,i,4} & c_{14,i,4} & c_{15,i,4} & & & \\ & & & \ddots & & & & & \\ & & & c_{11,i,2n-3} & c_{12,i,2n-3} & c_{13,i,2n-3} & c_{14,i,2n-3} & c_{15,i,2n-3} & \\ & & & & c_{11,i,2n-2} & c_{12,i,2n-2} & c_{13,i,2n-2} & c_{14,i,2n-2} & c_{15,i,2n-2} \\ & c_{15,i,2n-1} & & & & c_{11,i,2n-1} & c_{12,i,2n-1} & c_{13,i,2n-1} & c_{14,i,2n-1} \\ -6 & 4 & -1 & & & & -1 & 4 & \end{pmatrix}, \tag{12}$$

$$\mathbf{U}_{4,i} = \begin{pmatrix} 0 & & & & & & & & 0 \\ c_{17,i,2} & c_{18,i,2} & c_{19,i,2} & c_{20,i,2} & & & & c_{16,i,2} & \\ c_{16,i,3} & c_{17,i,3} & c_{18,i,3} & c_{19,i,3} & c_{20,i,3} & & & & \\ & c_{16,i,4} & c_{17,i,4} & c_{18,i,4} & c_{19,i,4} & c_{20,i,4} & & & \\ & & & \ddots & & & & & \\ & & & c_{16,i,2n-3} & c_{17,i,2n-3} & c_{18,i,2n-3} & c_{19,i,2n-3} & c_{20,i,2n-3} & \\ & & & & c_{16,i,2n-2} & c_{17,i,2n-2} & c_{18,i,2n-2} & c_{19,i,2n-2} & c_{20,i,2n-2} \\ & c_{20,i,2n-1} & & & & c_{16,i,2n-1} & c_{17,i,2n-1} & c_{18,i,2n-1} & c_{19,i,2n-1} \\ 0 & & & & & & & & 0 \end{pmatrix}, \tag{13}$$

$$\mathbf{U}_{5,i} = \begin{pmatrix} 0 & & & & & & & & 0 \\ c_{22,i,2} & c_{23,i,2} & c_{24,i,2} & c_{25,i,2} & & & & c_{21,i,2} & \\ c_{21,i,3} & c_{22,i,3} & c_{23,i,3} & c_{24,i,3} & c_{25,i,3} & & & & \\ & c_{21,i,4} & c_{22,i,4} & c_{23,i,4} & c_{24,i,4} & c_{25,i,4} & & & \\ & & & \ddots & & & & & \\ & & & c_{21,i,2n-3} & c_{22,i,2n-3} & c_{23,i,2n-3} & c_{24,i,2n-3} & c_{25,i,2n-3} & \\ & & & & c_{21,i,2n-2} & c_{22,i,2n-2} & c_{23,i,2n-2} & c_{24,i,2n-2} & c_{25,i,2n-2} \\ & c_{25,i,2n-1} & & & & c_{21,i,2n-1} & c_{22,i,2n-1} & c_{23,i,2n-1} & c_{24,i,2n-1} \\ 0 & & & & & & & & 0 \end{pmatrix}. \tag{14}$$

The elements $c_{1,i,j}$, $c_{2,i,j}$, ..., $c_{25,i,j}$ are the coefficients of the discretized equations of Eq. 6. Considering Eq. 9, the ranges of the index i for $\mathbf{U}_{1,i}$, $\mathbf{U}_{2,i}$, $\mathbf{U}_{3,i}$, $\mathbf{U}_{4,i}$ and $\mathbf{U}_{5,i}$ are $4 \to 2n-1$, $3 \to 2n-1$, $2 \to 2n-1$, $2 \to 2n-2$ and $2 \to 2n-3$, respectively. The range of the index j for the elements in $\mathbf{U}_{l,i}$ is from 2 to $2n-1$. We can find the dimension of $\mathbf{U}$ as follows: each matrix of the form $\mathbf{U}_{3,i}$ is of order 2n; the main diagonal consists of matrices of the form $\mathbf{U}_{3,i}$ and there are $2n-2$ of them (the range of the index i for $\mathbf{U}_{3,i}$ is $2 \to 2n-1$), the dimension of $\mathbf{U}$ is thus $(2n-2)2n \times (2n-2)2n$.

The boundary conditions of Eq. 7 have been incorporated into $\mathbf{U}$: the periodic condition of Eq. 7a is explicitly expressed in all the first rows of $\mathbf{U}_{3,i}$ (see Eq. 12); the derivative condition of Eq. 7b is treated by the four-point difference techniques in all the last rows of $\mathbf{U}_{3,i}$; the zero condition of Eq. 7c is implemented at $i = 1, 2n$, which is the reason that the range of the index i for $\mathbf{U}_{3,i}$ is from 2 to $2n-1$. The zero solutions on and outside the boundaries at $i = 1, 2n$ also lead to the structures of the first and last two rows in $\mathbf{U}$ (see Eq. 9).

Except for the first and last rows, all the other rows

in $\mathbf{U}_{l,i}$ have the same structure. In the second and second last rows of $\mathbf{U}_{l,i}$, the periodic property of the solutions is considered. As exemplified in the second last rows of $\mathbf{U}_{l,2n-1}$ ($l = 1, 2, 3, 4, 5$), the five coefficients $c_{5,2n-1,2n-1}$, $c_{10,2n-1,2n-1}$, $c_{15,2n-1,2n-1}$, $c_{20,2n-1,2n-1}$ and $c_{25,2n-1,2n-1}$ are there (cf. Eqs. 10-14) because the discrete solutions corresponding to these coefficients are equivalent to the counterparts at $j = 2$.

For non-trivial solutions, the determinant of $\mathbf{U}$ should be zero,

$$\det|\mathbf{U}| = 0. \tag{15}$$

By eliminating the constant elements in the first and last rows (columns) in the matrices $\mathbf{U}_{3,i}$, namely, eliminating the first and last rows (columns) in $\mathbf{U}_{l,i}$, Eq. 15 can be transformed into

$$\det|\mathbf{U}'| = 0, \tag{16}$$

where the block matrices $\mathbf{U}'_{l,i}$ ($l = 1, 2, 3, 4, 5$ and i is the counterpart subscript in $\mathbf{U}_{l,i}$) in $\mathbf{U}'$ have the following general structure,

$$\mathbf{U}'_{l,i} = \begin{pmatrix} \epsilon_2 + \frac{2}{3}\nu_2 & \sigma_2 - \frac{1}{6}\nu_2 & \tau_2 & & & & & & & -\frac{1}{6}\nu_2 & & \mu_2 + \frac{2}{3}\nu_2 \\ \nu_3 + \frac{2}{3}\mu_3 & \epsilon_3 - \frac{1}{6}\mu_3 & \sigma_3 & \tau_3 & & & & & & -\frac{1}{6}\mu_3 & & \frac{2}{3}\mu_3 \\ \mu_4 & \nu_4 & \epsilon_4 & \sigma_4 & \tau_4 & & & & & & & \\ & \mu_5 & \nu_5 & \epsilon_5 & \sigma_5 & \tau_5 & & & & & & \\ & & & & \ddots & & & & & & & \\ & & & & & \mu_{2n-4} & \nu_{2n-4} & \epsilon_{2n-4} & \sigma_{2n-4} & \tau_{2n-4} & & \\ & & & & & & \mu_{2n-3} & \nu_{2n-3} & \epsilon_{2n-3} & \sigma_{2n-3} & & \tau_{2n-3} \\ \frac{2}{3}\tau_{2n-2} & -\frac{1}{6}\tau_{2n-2} & & & & & & \mu_{2n-2} & \nu_{2n-2} & \epsilon_{2n-2} - \frac{1}{6}\tau_{2n-2} & \sigma_{2n-2} + \frac{2}{3}\tau_{2n-2} \\ \tau_{2n-1} + \frac{2}{3}\sigma_{2n-1} & -\frac{1}{6}\sigma_{2n-1} & & & & & & & \mu_{2n-1} & \nu_{2n-1} - \frac{1}{6}\sigma_{2n-1} & \epsilon_{2n-1} + \frac{2}{3}\sigma_{2n-1} \end{pmatrix}. \tag{17}$$

As a matter of convenience, the notations l, i are omitted in the elements above and only the index j ($j = 2, 3, ..., 2n - 1$) is given. The quantities of $\mu(l)_{i,j}$, $\nu(l)_{i,j}$, $\epsilon(l)_{i,j}$, $\sigma(l)_{i,j}$ and $\tau(l)_{i,j}$ indicate the corresponding elements from $\mathbf{U}$. For example, ϵ_j in $\mathbf{U}'_{3,i}$ is $\epsilon(3)_{i,j} \leftrightarrow c_{13,i,j}$ in $\mathbf{U}_{3,i}$; μ_4 in $\mathbf{U}'_{1,i}$ is $\mu(1)_{i,4} \leftrightarrow c_{1,i,4}$ in $\mathbf{U}_{1,i}$; μ_4 in $\mathbf{U}'_{2,i}$ is $\mu(2)_{i,4} \leftrightarrow c_{6,i,4}$ in $\mathbf{U}_{2,i}$; μ_4 in $\mathbf{U}'_{3,i}$ is $\mu(3)_{i,4} \leftrightarrow c_{11,i,4}$ in $\mathbf{U}_{3,i}$. Each $\mathbf{U}'_{l,i}$ is of order $2n - 2$. Thus, the dimension of $\mathbf{U}'$ is $(2n-2)(2n-2) \times (2n-2)(2n-2)$, which is less than that of $\mathbf{U}$.

It can be verified that the parameters of the magnetic field B, contained in the $c_{13,i,j}$ coefficients, only appear in the main diagonal position of $\mathbf{U}$ (thus $\mathbf{U}'$). Since $c_{13,i,j}$ can be categorized into two different parts: with and without B, Eq. 16 can be further written as

$$\det|\mathbf{P} - B^2\mathbf{I}| = 0, \tag{18}$$

where $\mathbf{I}$ is a unitary matrix. $\mathbf{P}$ has the same structure and dimension as $\mathbf{U}'$ and the block matrices $\mathbf{P}_{l,i}$ in $\mathbf{P}$ have the following general structure,

$$\mathbf{P}_{l,i} = \begin{pmatrix} \epsilon'_2 + \frac{2}{3}\nu_2 & \sigma_2 - \frac{1}{6}\nu_2 & \tau_2 & & & & & & & -\frac{1}{6}\nu_2 & & \mu_2 + \frac{2}{3}\nu_2 \\ \nu_3 + \frac{2}{3}\mu_3 & \epsilon'_3 - \frac{1}{6}\mu_3 & \sigma_3 & \tau_3 & & & & & & -\frac{1}{6}\mu_3 & & \frac{2}{3}\mu_3 \\ \mu_4 & \nu_4 & \epsilon'_4 & \sigma_4 & \tau_4 & & & & & & & \\ & \mu_5 & \nu_5 & \epsilon'_5 & \sigma_5 & \tau_5 & & & & & & \\ & & & & \ddots & & & & & & & \\ & & & & & \mu_{2n-4} & \nu_{2n-4} & \epsilon'_{2n-4} & \sigma_{2n-4} & \tau_{2n-4} & & \\ & & & & & & \mu_{2n-3} & \nu_{2n-3} & \epsilon'_{2n-3} & \sigma_{2n-3} & & \tau_{2n-3} \\ \frac{2}{3}\tau_{2n-2} & -\frac{1}{6}\tau_{2n-2} & & & & & & \mu_{2n-2} & \nu_{2n-2} & \epsilon'_{2n-2} - \frac{1}{6}\tau_{2n-2} & \sigma_{2n-2} + \frac{2}{3}\tau_{2n-2} \\ \tau_{2n-1} + \frac{2}{3}\sigma_{2n-1} & -\frac{1}{6}\sigma_{2n-1} & & & & & & & \mu_{2n-1} & \nu_{2n-1} - \frac{1}{6}\sigma_{2n-1} & \epsilon'_{2n-1} + \frac{2}{3}\sigma_{2n-1} \end{pmatrix}, \tag{19}$$

where ϵ'_j is short for $\epsilon'(l)_{i,j}$ and one has

$$\epsilon'(l)_{i,j} = \begin{cases} \epsilon(l)_{i,j} & l = 1, 2, 4, 5 \\ \epsilon(l)_{i,j} - B^2 & l = 3. \end{cases} \tag{20}$$

Thus, $\mathbf{P}_{l,i}|_{l=1,2,4,5} = \mathbf{U}'_{l,i}|_{l=1,2,4,5}$ but $\mathbf{P}_{3,i} \neq \mathbf{U}'_{3,i}$.

From Eq. 18, it is clear that the largest solution for B, namely B_{c2}, can be obtained from the maximum eigenvalue of the following eigen equation,

$$\mathbf{P}\chi = B^2\chi, \tag{21}$$

where χ is the eigen function of $\mathbf{P}$. Having obtained B_{c2}, the corresponding order parameter can be obtained by substituting B_{c2} into Eq. 8.

B. Procedure II

In the above procedure, the magnetic field square B^2 has been treated as an eigenvalue (Eq. 21). In fact, one can directly discretize Eq. 6 into a matrix eigen equation, from which the upper critical field can be directly deduced,

$$\mathbf{Q}\boldsymbol{\Phi} = B^2\boldsymbol{\Phi}, \qquad (22)$$

where the matrix $\mathbf{Q}$ has the same structure as $\mathbf{U}$ and the block matrices in $\mathbf{Q}$ have the following general structure,

$$\mathbf{Q}_{l,i} = \begin{pmatrix} \epsilon'_1 & \sigma_1 & \tau_1 & & & & & & \mu_1 & \nu_1 \\ \nu_2 & \epsilon'_2 & \sigma_2 & \tau_2 & & & & & & \mu_2 \\ \mu_3 & \nu_3 & \epsilon'_3 & \sigma_3 & \tau_3 & & & & & \\ & \mu_4 & \nu_4 & \epsilon'_4 & \sigma_4 & \tau_4 & & & & \\ & & & & \ddots & & & & & \\ & & & & \mu_{2n-3} & \nu_{2n-3} & \epsilon'_{2n-3} & \sigma_{2n-3} & \tau_{2n-3} & \\ & & & & & \mu_{2n-2} & \nu_{2n-2} & \epsilon'_{2n-2} & \sigma_{2n-2} & \tau_{2n-2} \\ & \tau_{2n-1} & & & & & \mu_{2n-1} & \nu_{2n-1} & \epsilon'_{2n-1} & \sigma_{2n-1} \\ & \sigma_{2n} & \tau_{2n} & & & & & \mu_{2n} & \nu_{2n} & \epsilon'_{2n} \end{pmatrix}. \qquad (23)$$

Here, the quantities of μ_j, ν_j, ϵ'_j, σ_j and τ_j have the same meaning as those in $\mathbf{P}_{l,i}$. Unlike that in $\mathbf{U}_{l,i}$, $\mathbf{U}'_{l,i}$ and $\mathbf{P}_{l,i}$, the range of the index j in $\mathbf{Q}_{l,i}$ is now from 1 to $2n$. The dimension of $\mathbf{Q}$ is the same as that of $\mathbf{U}$, i.e., $(2n-2)2n \times (2n-2)2n$. Note that the periodic property of the solutions has been considered implicitly in the first and last rows of $\mathbf{Q}_{l,i}$, unlike the explicit condition in $\mathbf{U}_{3,i}$ (see Eq. 12). Such a periodic property also appears in the second and last second rows in $\mathbf{Q}_{l,i}$ as well as in $\mathbf{U}_{l,i}$.

The present procedure allows a direct determination of the upper critical field from the largest eigenvalue of the magnetic field square of the linear GL equation, compared to the conventional method that B_{c2} is obtained via the lowest eigenvalue of the Landau level of the linear GL equation[1,9–15].

IV. RESULTS AND DISCUSSION

In the above procedures, we have treated the magnetic field square as eigenvalue problems (Eq. 21 and Eq. 22) and hence, the upper critical field in the c-a plane can be directly obtained from the corresponding eigen equations. It should be noted that these procedures are related to the partial differential Eq. 6, namely a 2D differential equation. Note that we can have similar procedures to determine the upper critical field parallel to the layers[3] but these procedures (corresponding to Eqs. 5 and 6 in Ref. 3, respectively) are now related to an ordinary differential equation, i.e., a 1D differential equation (see Eq. 1 in Ref. 3). The values of B_{c2} of Bi2212, calculated from the two 2D procedures under the conditions of $\theta = 89.9°$ and $T = 0$ K, are presented in Table I. The corresponding 1D calculations at $\theta = 90°$ and $T = 0$ K are also listed. It can be seen that the results obtained from the 2D procedures ($\theta = 89.9°$) are in good agreement with each other and reasonably approximate the corresponding 1D calculations ($\theta = 90°$).

It is found that the order parameter obtained at B_{c2} from procedure I (Eq. 21) is also consistent with that from procedure II (Eq. 22) and we shall utilize procedure II for the following calculations. In Fig. 1, we show the surface and contour plots of the order parameter for Bi2212 with the conditions $\theta = 89.9°$ and $T = 0$ K. Note that the x'-axis nearly overlaps the z- (c-) axis (namely, $x' \approx z$) at $\theta = 89.9°$. Hence, as depicted in Fig. 1, the order parameter of Bi2212 is localized in a thin slab ($z \in [-2, 2]$ a.u.) along the c- axis. The behavior found here is consistent with the fact that for Bi2212 the c-axis coherence length at zero temperature is very short[16] and less than the distance between the two effective superconducting layers (~ 12.34 Å, see Ref. 3). However, for another intrinsically layered superconductor YBCO with relatively small anisotropy[17], we found that the localized domain at zero temperature is about $z \in [-10, 10]$ a.u., which is broader than the distance between the two effective superconducting layers (~ 8.41 Å, see Ref. 3). As such, one may say that at zero temperature, Bi2212 exhibits a 2D feature while YBCO demonstrates a quasi-3D behavior.

Fig. 2 shows the order parameter and its contour at B_{c2} for Bi2212 at a higher temperature $0.9\,T_c$, with the angle $\theta = 89.9°$ unchanged. It is obvious that the order parameter becomes broader than the case at zero temperature (Fig. 1), as expected. The localized domain across the layer is now about $z \in [-6, 6]$ a.u. and it is still smaller than the distance between the adjacent superconducting layers. This behavior is qualitatively consistent with the 2D feature of Bi2212 at $0.9\,T_c$ calculated by the one-dimensional procedure. However, for YBCO, we find that the localized domain at $0.9\,T_c$ is about $z \in [-15, 15]$ a.u., larger again than the distance between the nearest superconducting layers. Consequently, one may conclude that Bi2212 is a 2D superconductor in a large temperature while YBCO is intrinsically a quasi-3D superconductor. Note that the order parameter presented in Figs. 1 and 2 are found to be of a Gaussian type, which is consistent with the fact that the profile of the order parameter associated with the smallest eigenvalue (Landau level) of the usual linear GL equation at B_{c2}.

Finally, it is worth mentioning that Eq. 21 of procedure I requires less memory than Eq. 22 of procedure II in obtaining B_{c2} since the dimension of $\mathbf{P}$ is less than that of $\mathbf{Q}$. The number of the stored elements in the sparse matrix $\mathbf{P}$ is less than that in $\mathbf{Q}$ by

$(2n-2)2n \times (2n-2)2n - (2n-2)(2n-2) \times (2n-2)(2n-2) = 16(2n-1)(n-1)^2$. When n is large, the reduced amount ($\approx 32n^3$) is significant. However, in order to obtain both B_{c2} and the associated order parameter, procedure I requires more CPU time than procedure II since in using procedure I, two equations (Eqs. 8 and 21) have to be solved while only one equation (Eq. 22) is involved in procedure II.

V. CONCLUSION

In this paper, we applied our continuous Ginzburg-Landau model to layered superconductors in the presence of a magnetic field parallel to the c-a plane. By treating the magnetic field square as eigenvalues, two procedures were proposed to determine the upper critical field. Near the direction parallel to the layers, the critical fields of Bi2212 calculated from the two procedures are consistent with each other and are good approximations to the corresponding parallel upper critical fields determined by similar procedures. The behaviors of the order parameter obtained at B_{c2} are reasonable. Our procedures can be a useful starting point for investigating the properties associated with the upper critical field and the corresponding order parameter.

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TABLE I. Values of B_{c2} (Tesla) at $89.9°$ at 0 K for Bi2212, determined by the two 2D procedures (Eq. 21 and Eq. 22). The results from the 2D procedures are consistent with each other and reasonably approximate the parallel upper critical fields determined by the corresponding 1D procedures.

procedure	n	B_{c2}
	30	3342.3065
I (2D, Eq. 21)	40	3337.3166
	50	3336.7392
I (1D)	800	3338.6584
	30	3338.7414
II (2D, Eq. 22)	40	3336.9549
	50	3336.8420
II (1D)	800	3338.6801

FIG. 1. Surface and contour plots of the order parameter of Bi2212 at zero temperature. The plots are depicted against the z'-x' plane (x' is from negative to positive and z' is from 5000 to 12000). The order parameter is localized in a narrow domain (about 6. a.u.) along the c-axis unit cell.

FIG. 2. Surface and contour plots of the order parameter of Bi2212 at 0.9 T_c. The order parameter spreads out and becomes broader than that at zero temperature (see Fig. 1).
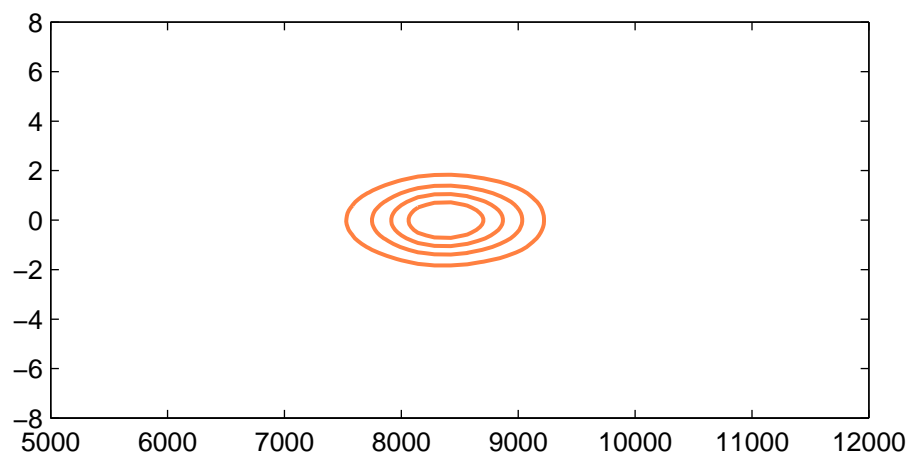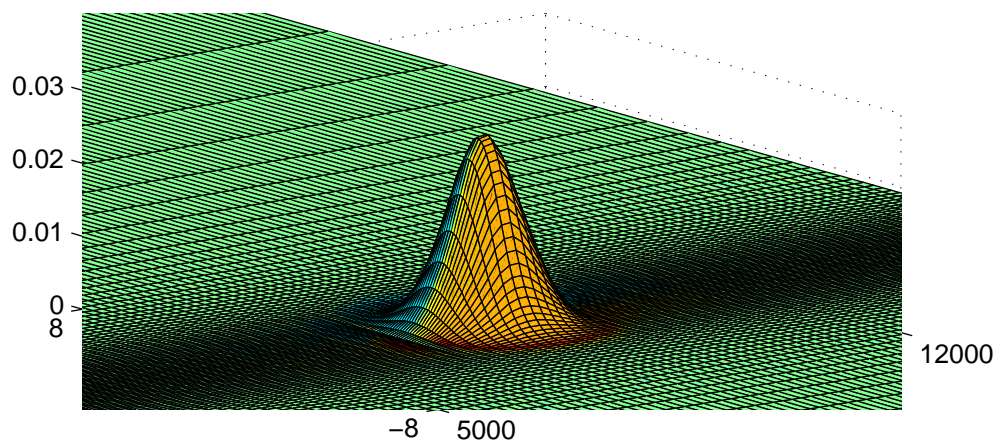
Figure 1

Figure 2